1,3-Dioxolane 646-06-0 | DTXSID4027284

Model	Performance	
MOUC	renomiance	

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 6.47 days

Global applicability domain: Outside

Local applicability domain index: 3.48e-01

Confidence level: 8.78e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 40.7 **Predicted:** 6.52

Image not found

n-Hexane

Measured: 157 Predicted: 7.45

Image not found

Heptane

Measured: 88.3 **Predicted:** 7.54

Image not found

Hexane, 2,2-dimethyl-

Measured: 24.3 Predicted: 4.47 Image not found

Octane

Measured: 157 Predicted: 8.57